Spectral beam attenuation coefficient retrieved from ocean color inversion

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[1] A reflectance inversion model in presented in which particle backscattering is parameterized by the particle backscattering ratio, attenuation and absorption coefficients rather than a hyperbolic function. This parameterization removes backscattering spectral constraints and yields independent estimates of the magnitude and spectral slope of the particle beam attenuation, which have been found to correlate with the particle concentration and size distribution, respectively. The model yields estimates of component absorption and backscattering consistent with observations and Mie models, particularly for environments dominated by phytoplankton and other strongly absorbing particles. *INDEX TERMS:* 4552 Oceanography: Physical: Ocean optics; 4847 Oceanography: Biological and Chemical: Optics; 4275 Oceanography: General: Remote sensing and electromagnetic processes (0689). **Citation:** Roesler, C. S., and E. Boss, Spectral beam attenuation coefficient retrieved from ocean color inversion, *Geophys. Res. Lett.*, *30*(9), 1468, doi:10.1029/2002GL016185, 2003.

1. Introduction

[2] Ocean color contains a wealth of information regarding the concentration and composition of dissolved and suspended constituents in the sea. Analytic expressions derived from simplifications to the radiative transfer equation express the radiance and irradiance reflectance as a function of the inherent optical properties (IOPs) [e.g., *Gordon et al.*, 1988]:

$$R = G\frac{b_b}{a + b_b} \tag{1}$$

where R is reflectance (ratio of upward irradiance or radiance to the downward irradiance), G depends upon the definition of R and water and atmospheric properties, and a and b_b are absorption and backscattering coefficients.

[3] Semi-analytical inversion models extract constituent IOPs from measured reflectance signatures [*Gordon et al.*, 1988; *Lee et al.*, 1994; *Roesler and Perry*, 1995; *Hoge and Lyon*, 1996, 1999; *Garver and Siegel*, 1997]. The IOPs are linearly deconvolved into operational components and expressed as the product of scalar amplitudes and non-dimensionalized basis functions (spectra):

$$a = a_w + L_\varphi\,\hat{a}_\varphi + L_{CPM}\,\hat{a}_{CPM} + L_{CDM}\,\hat{a}_{CDM} \tag{2a}$$

$$b_b = b_{bw} + L_{bbp}\,\hat{b}_{bp} \tag{2b}$$

where the subscripts w, p, φ, CPM and CDM indicate water, total particles, phytoplankton, colored particulate material (exclusive of phytoplankton), and colored dissolved material, amplitudes are indicated by L, and basis functions by ^.

[4] Published inversion models differ in basis function definitions and solution methods. Decades of laboratory and field investigations yield robust constraints on the absorption basis function spectral variations. Backscattering sensors are relatively new and there is less information on backscattering basis functions. Observations and Mie theory for absorbing spheres yield strong spectral features near absorption peaks [*van de Hulst*, 1957; *Gordon*, 1974; *Bricaud and Morel*, 1986; *Zaneveld and Kitchen*, 1995]. Difficulty in constraining these features has lead to implementation of Mie theory for populations of *non-absorbing* homogeneous spheres, in which b_{bp} is expressed as a smoothly varying function [*Morel*, 1973]:

$$b_{bp}(\lambda) = b_{bp}(\lambda_o)\left(\frac{\lambda}{\lambda_o}\right)^{\eta} \tag{3}$$

where λ is wavelength, λ_o is a nominal scaling wavelength, and η is the hyperbolic slope (which is either held constant or retrieved by inversion).

[5] The utility of such models has been demonstrated over a range of environments, particularly for estimation of a_φ and the combined $a_{CPM+CDM}$, with less confidence in derived b_{bp} values. In this paper, we propose to build upon this background to develop an algorithm that removes spectral constraints on b_{bp} by allowing the influence of a_p on b_{bp} to be parameterized. This is achieved by using IOP observations and theory to expand the inversion algorithm and in doing so retrieve estimates of the spectral particle beam attenuation coefficient and the particle backscattering ratio.

2. Model Development and Tests

[6] The focus of this model relies on replacing the expression for b_{bp} given by (3), in which we have relatively

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little confidence, by a function in whose spectral shape we have a good deal of confidence. We express the particle backscattering spectrum as:

$$b_{bp}(\lambda) = \tilde{b}_{bp}(\lambda) b_p(\lambda) \quad (4)$$

where $\tilde{b}_{bp}$ is the particle backscattering ratio (defined as the backscattering to total scattering ratio), and b_p is the particle scattering spectrum. Mie theory predicts spectrally independent backscattering ratios for Junge populations of absorbing particles with constant real refractive indices [*Ulloa et al.*, 1994]. Although some spectral variations are observed for monospecific phytoplankton cultures [*Stramski and Mobley*, 1997], in situ observations on limited data sets suggest they are weak (<10% [*Twardowski et al.*, 2001]). Assuming no spectral dependence in the backscattering ratio and recognizing that b_p can be expressed by the difference between particle attenuation, c_p, and absorption, a_p, yields:

$$b_{bp}(\lambda) = \tilde{b}_{bp}\left[c_p(\lambda) - \left(a_j(\lambda) + a_{CDM}(\lambda)\right)\right]. \quad (5)$$

[7] Unlike the spectral dependence of b_{bp}, c_p is observed to be a smoothly varying function of wavelength, even for strongly absorbing particle populations [*Voss*, 1992; *Barnard et al.*, 1998; *Boss et al.*, 2001a], and is well described by:

$$c_p(\lambda) = c_p(\lambda_0)\left(\frac{\lambda}{\lambda_0}\right)^{\gamma} \quad (6)$$

where γ is the hyperbolic slope. Mie solutions for c_p show small departures from (6) for hyperbolically distributed absorbing particles (<2%) [*Boss et al.*, 2001b]. We define the c-model for inversion (c as in attenuation) by (1) with F/Q replaced by the estimable amplitude $L_{F/Q}$, a given by (2a) and:

$$b_b = b_{bw} + L_{\tilde{b}_{bp}}\left[L_{cp}\left(\frac{\lambda}{\lambda_0}\right)^{-L\gamma} - L_{\varphi}\hat{a}_{\varphi} - L_{CPM}\hat{a}_{CPM}\right]. \quad (7)$$

The basis functions are defined a priori and amplitudes, L, are estimated by optimization. The spectral restriction on b_{bp}, as defined by (3), is replaced by two functions, $\tilde{b}_{bp}$ and c_p, which have minimal or well-constrained spectral dependences.

[8] We solve the inversion with a bounded non-linear least squares minimization (Levenberg-Marquard [*Press et al.*, 1989]). Without bounds, >1 minima can be found over a three-order dynamic range yielding negative/non-physical solutions. We define a priori three overlapping ranges of upper and lower amplitude bounds (where each range spans over a factor of 10) based upon environment: open ocean, coastal and extreme blooms. For example, the amplitude bounds for L_{cp} are 0.03–0.3, 0.1–1, and 0.8–8.

[9] The amplitude $L_{F/Q}$ is allowed to vary within the entire F/Q range observed by *Morel and Gentili* [1996], but not spectrally, although is has been shown to have spectral variations [*Morel et al.*, 2002]. As we gain more understanding of the spectral variations, this factor can become a basis function in the model. Water backscattering [*Morel*, 1974] and absorption [*Pope and Fry*, 1997] are corrected for in situ temperature and salinity conditions [*Morel*, 1974; *Pegau et al.*, 1997]. The basis functions for $\hat{a}_{CDM}$ and $\hat{a}_{CPM}$ are defined by exponential functions with slopes of −0.018 and −0.011 nm^{-1}, respectively [*Roesler et al.*, 1989]. For simplicity, the phytoplankton basis function, $\hat{a}_{\varphi}$, is defined by an average spectrum [*Roesler and Perry*, 1995, Figure 1], although using multiple functions for each pigment-based taxonomic groups improves reflectance fit and yields taxonomic information (C. S. Roesler et al., Application of an ocean color algal taxa detection model to the red tide communities of the southern Benguela, submitted to *Proceedings of the 10th International Conference on Harmful Algal Blooms*, 2003).

[10] C-model results are compared first to those derived from the published model of *Roesler and Perry* [1995] (referred to here as the *standard model*). Identical basis functions were used for the $\hat{a}$ components in both models. In the standard model b_{bp} was parameterized by the sum of 2 basis functions defined by (3) with η = 0 and −1, respectively.

[11] Amplitudes from the c-model were then compared with measured values collected over a broad range of optical domains: clear gyre waters off the Oregon coast, coastal Gulf of Maine (GoM) and Benguelan Upwelling waters, some with extreme algal bloom conditions. Observed a_p, a_{CDM}, and c_p spectra were derived from in situ ac9 measurements using simultaneous filtered (0.2-μm) and unfiltered configurations, with corrections as in *Roesler* [1998], or as in *Roesler and Perry* [1995] for gyre stations. The spectral slope, γ, was derived by non-linear least-squares regression of (6) onto c_p observations. b_{bp} coefficients were measured with a WETLabs ECOvsf, calibrated with beads and corrected for variable path absorption. There were no backscattering measurements from the gyre and GoM stations, so b_{bp} and $\tilde{b}_{bp}$ were determined from *Petzold* [1972] using data from Bermuda (AUTEC) and offshore southern California (HAOCE), respectively, which had absorption and attenuation coefficients within 10% of our measured values.

[12] Hyperspectral surface reflectance was measured with either a LICOR 1800UW scanning radiometer [*Roesler and Perry*, 1995] or a Satlantic H-TSRB radiometer buoy. Upwelling measurements were corrected to the surface using spectral attenuation coefficients measured in the top meter.

3. Results

[13] Chlorophyll values ranged from 0.07 to 131.65 μg/L. Reflectance spectra were well predicted by both models although the c-model yielded better fits (Figures 1A and 1B). The spectral shape of b_{bp} was better predicted by the c-model, with the standard model often yielding unrealistic spectra (e.g., negative values, Figures 1C and 1D). The c-model provided significantly better estimates of a_p and a_{CDM} amplitude and spectral shape (Figures 1E–1H). In general, the standard model overestimated all the IOP components in the blue.

[14] C-modeled amplitudes were linearly correlated with observed values (Figure 2) and these relationships are expressed by the slope (m) and intercept (i). The observa-

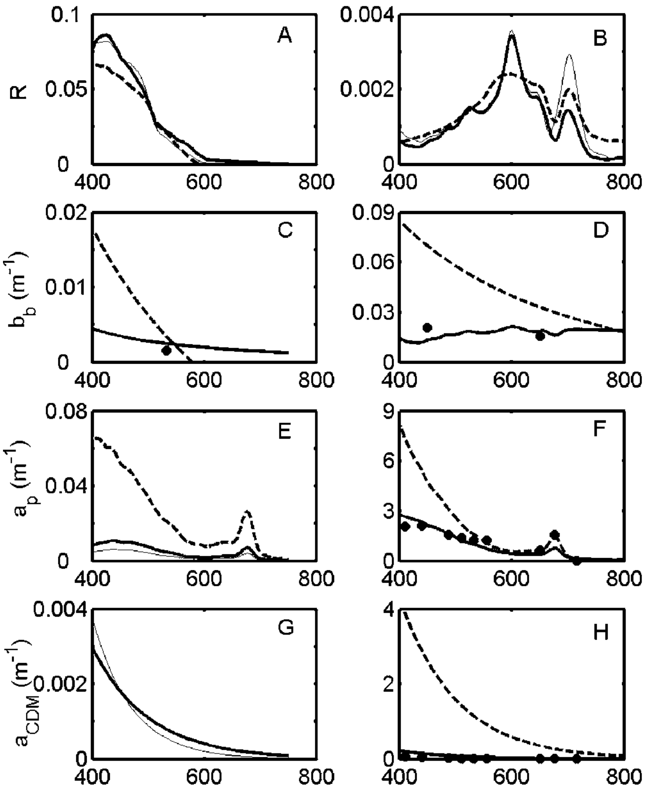

Figure 1. Observed and modeled parameters for two optically diverse regimes: spectral reflectance (A, irradiance, and B, radiance, reflectance), backscattering (C, D), particulate absorption (E, F) and CDM absorption (G, H). Observations were made in the gyre waters off the Oregon coast (left panels) and Benguelan coastal waters off South Africa (right panels). Chlorophyll values were 0.07 and 131.65 μg/L, respectively. Observed values are thin black lines or symbols, values from the standard model are bold solid lines, and from c-model are bold dash lines.

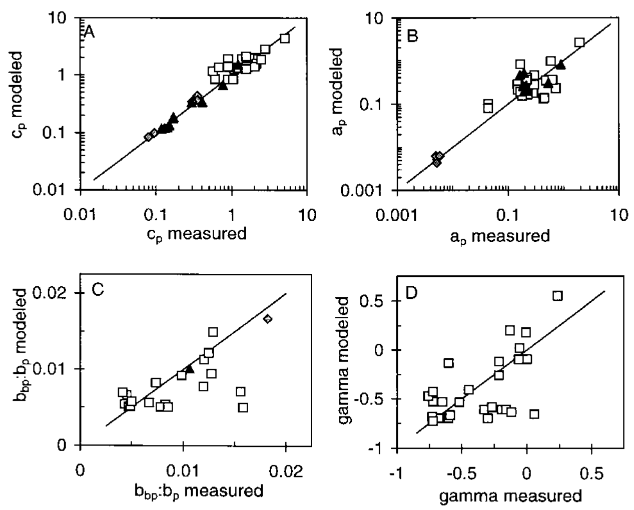

Figure 2. Measured vs. modeled optical properties: particulate attenuation (A) and absorption coefficients (B) at 440nm, particulate backscattering ratio at 650nm (C; 532 nm for gyre and GoM), and slope of the particulate attenuation spectrum (γ, D). Symbols: gyre - gray diamond, Gulf of Maine - black triangle, Benguela Upwelling - open square.

tions span a large dynamic range and because correlation coefficients are driven by range and not localized fit, the mean absolute deviation (mad) of retrieved estimates about the linear fit is a robust estimator of goodness-of-fit [*Press et al.*, 1989] (Table 1). C-modeled $c_p(440)$ and $a_p(440)$ estimates were highly correlated with observed values. Correlations were not as strong for the particle backscattering ratio, but improved when two observations associated with dominance by large detrital organic particles are excluded (0.77, 0.001, 0.001 for m, i, mad, respectively). C-modeled estimates of c_p slope, γ, had the weakest correlation, particularly for cases where particles were dominated by very high concentrations of large (>20 μm) algal cells. The fit improved significantly without them (1.01, 0.11, 0.10 for m, i, mad, respectively).

4. Discussion

[15] The importance of obtaining more than chlorophyll from ocean color has lead to the development of many inversion algorithms. Enhanced spectral resolution of remote and in situ radiometers has expanded the capability for retrieving not only more components by inversion, but improved spectral information associated with those components. Regardless, published inversion models have yet to remove the constraints on particle backscattering spectra. In this paper we present an inversion algorithm in which the spectral constraints on the particle backscattering are removed and placed on the particle attenuation coefficient and the backscattering ratio, two parameters with better-established spectral dependences [*Voss*, 1992; *Barnard et al.*, 1998; *Boss et al.*, 2001b]. The implicit assumption is that the same particles responsible for b_{bp} are responsible for c_p and a_p. Whereas theoretically, each IOP is differently dependent on particle size [*Stramski and Kiefer*, 1991; *Boss et al.*, 2001b], under most conditions it is likely that the same portions of the PSD will dominate all the IOPs, and in the open ocean, where small particles dominate, the IOPs and particles are well correlated. Future field, laboratory and modeling work will provide better constraints for these model assumptions.

[16] Under conditions where all optical properties are dominated by algal cells, we expect b_{bp} to vary predictably and in concert with a_p as has been documented for algal cultures. The c-model applied to extreme algal blooms yields these predictable backscattering spectral signatures that cannot be retrieved using a hyperbolic function for b_{bp}. The standard model did not provide as good b_{bp} spectra although it did fit the measured reflectance spectra reason-

Table 1. Slope, Intercept, and Mean Absolute Deviation (m, i, mad, respectively) of Modeled and Observed Amplitudes

Amplitude	Range	m	i	mad
$c_p(440)$	0.08–5.19	0.82	0.26	0.30
$a_p(440)$	0.005–1.935	1.02	−0.02	0.15
b_{bp}	0.004–0.018	0.57	0.003	0.002
γ	−0.76–0.24	0.68	−0.15	0.22

ably well. This was due to variance transference between b_{bp} and the CDM and CPM absorption basis functions. Variance transference is common in non-linear least squares problems in which exponentially (or hyperbolically) varying basis functions occur in both the numerator and the denominator. Minimization is achieved by a balance (sometimes unrealistic) between the two.

[17] An important achievement of the c-model is the estimate of c_p within 0.3 m^{-1} (average deviation 30%) over two orders of dynamic range. These results might be surprising given the lack of an analytic relationship between R and c (R is dominated by the small proportion of scattering that occurs at large angles, while c is dominated by the large proportion of scattering at the smallest angles [*Gordon*, 1993]), except that over a large dynamic range there is a first order relationship between backscattering and forward scattering driven by mass concentration. Higher order variations caused by PSD and the real refractive index, will be captured by $\tilde{b}_{bp}$, which is estimated with an average deviation of 17% (maximally 50%).

[18] This inversion does not depend on or constrain the relationship between c_p and b_{bp}, which are differently impacted by particle size and composition; in fact no relationship was observed in this data set. Thus, this model provides a significant improvement over empirical estimation of c_p from b_{bp} coefficients. Our interest in retrieving c_p from ocean color or surface reflectance lies in its strong correlation with particle volume and particulate organic carbon [*Spinrad*, 1986; *Bishop*, 1999].

[19] The poorest derived quantity from the c-model is the spectral slope of c_p, γ, although values were estimable within 0.22. Since γ is related linearly to the Junge slope of the PSD for most oceanic conditions [*Volz*, 1954; *Boss et al.*, 2001a, 2001b], retrieved values may be sufficient for qualitative estimates of PSD and ecosystem structure.

[20] Extending this model to remotely sensed ocean color data will require sensitivity analyses, incorporating uncertainty due to atmospheric correction and testing on multispectral data. However, the model in its current form is applicable to surface and near surface observations.

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